Simulation Overview
FLOORS
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Outline

- Modeling Overview
- Device Simulation Development
- Directions

FLOOPS / FLOODS / FLOORS

- Object-oriented codes
- Multi-dimensional
- P = Process / D = Device 90% code shared
- Scripting capability for PDE's - Alagator

- Commercialized - ISE / Synopsis
  - Sentaurus - Process is based on FLOOPS
- Licensed at over 400 sites world-wide
  - 2008 release
  - Manual is online (building a wiki manual)

What is Alagator?

- Scripting language for PDE's
- Parsed into an expression tree
- Assembled using FV / FE techniques
- Stored in hierarchical parameter data base

- Models are accessible, easily modified

What is Alagator?

Operator	*Description*
"ddt"	Time derivative
"grad"	Spatial derivative
"sgrad"	Scharfetter / Gummel Discretization Operator
"dot"	Returns the dot product of the gradient of two field – electric field in direction of current flow
"elastic"	Compute elastic forces - FEM balance

- Example use of operators for diffusion equation
- Fick's Second Law of Diffusion
  - ddt(Boron) - 9.0e-16 * grad(Boron) - K * (Boron - Trap)
  - $\partial C(x,t) / \partial t = D\, \partial^2 C(x,t) / \partial x^2 - K * C(x,t) * C_T$

Discretization – Current Density

Quasi-Fermi Current Density

$$J_n = -q\mu_n n \nabla \phi_n$$

$$J_p = -q\mu_p p \nabla \phi_p$$

Boltzmann Relations

$$\phi_n \equiv \psi - \frac{kT}{q}\ln(n/n_i)$$

$$\phi_p \equiv \psi + \frac{kT}{q}\ln(p/n_i)$$

Drift-Diffusion Current Density

$$J_n = qn\mu_n \mathrm{E} + qD_n \nabla n$$

$$J_p = qp\mu_p \mathrm{E} - qD_p \nabla p$$

- To obtain a closed system of equations, current densities written as function quasi-Fermi levels
- Using Boltzmann relations, current density can be written in the familiar relationship as the sum of drift and diffusion components

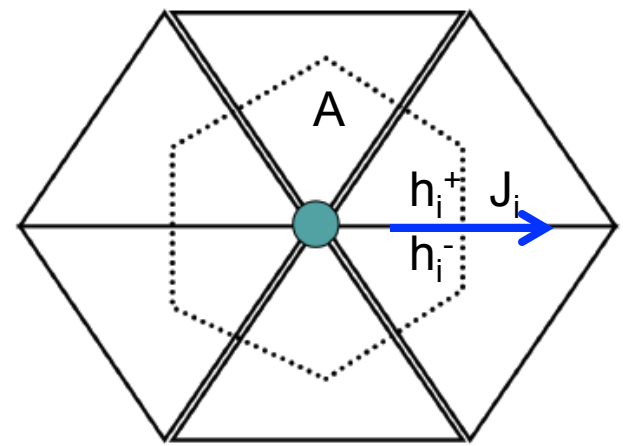
- Drift-Diffusion subtracting large numbers is not a good recipe with finite precision arithmetic

Finite Volume Scharfetter-Gummel (FVSG)

- Each PDE is integrated over a control volume *A*
- A is defined by the perpendicular bisectors of mesh elements
- PDe integrated using Green's formula
- Current $J_{n,p}$ evaluated using the Scharfetter-Gummel
- Scharfetter Gummel
  - Assume field and current constant
  - Solve resulting equation
  - $J_n/q = D\ (\ B(t)\ n_i+ - B(-t)\ n_i-\ )\ /\ l_i$
  - $t = \mu\ E\ /\ D$
  - $B(t) = t\ /\ (e^t - 1)$ Bernoulli Function

$$J_n = qn\mu_n \mathrm{E} + qD_n \nabla n$$

$$\frac{dn}{dt} = \frac{1}{q}\nabla \cdot J_n - U_n$$



$$\frac{1}{q}\sum_i J_i\left(h_i^+ + h_i^-\right) - A\left(U_n + \frac{dn}{dt}\right) = 0$$

- Advantages:
  - Commonly used "proven" method
  - Assembly time, each edge assembled once
- Disadvantages
  - Current defined only on edges, not continuous in space
  - Impact Ionization, Joule Heating more difficult
  - Works best when grid is aligned with current flow

Finite Element Quasi-Fermi (FEQF)

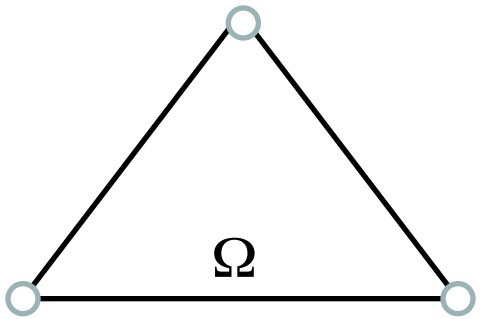
- $\phi_{n,p}$ defined at grid nodes
- Use shape function in an element
  - Piecewise linear most common
  - Can be higher order
- Integrate equations and minimize error

- Advantages:
  - Current is a continuous function over each element
  - Easier to compute Joule Heating, Impact Ionization
  - Compatible with strain calculations

- Disadvantages
  - Not as stable
  - Convergence issues

$$J_n = -q\mu_n n \nabla \varphi_n$$

$$\frac{dn}{dt} = \frac{1}{q}\nabla \cdot J_n - U_n$$



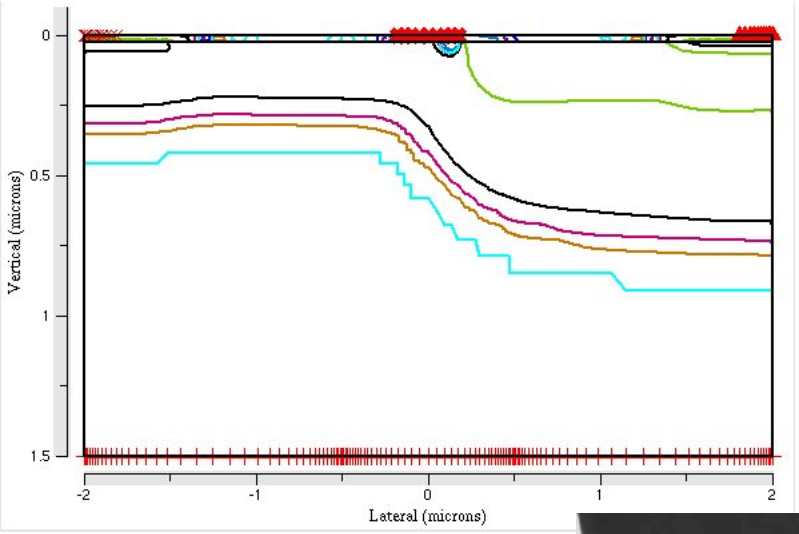
$$a(\psi, v) \equiv (-\rho, v)$$

$$a(\psi, v) \equiv \iint_{\Omega} \varepsilon \nabla \psi \cdot \nabla v \, dx \, dy$$

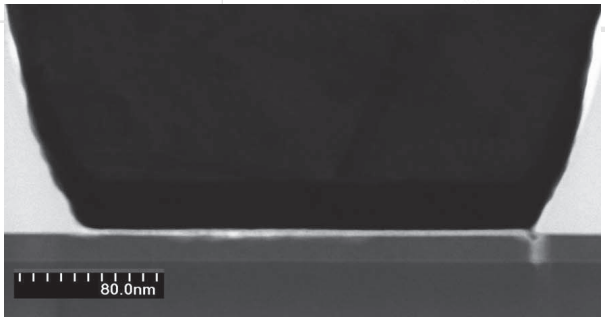
$$(-\rho, v) \equiv -\iint_{\Omega} \rho \, v \, dx \, dy$$

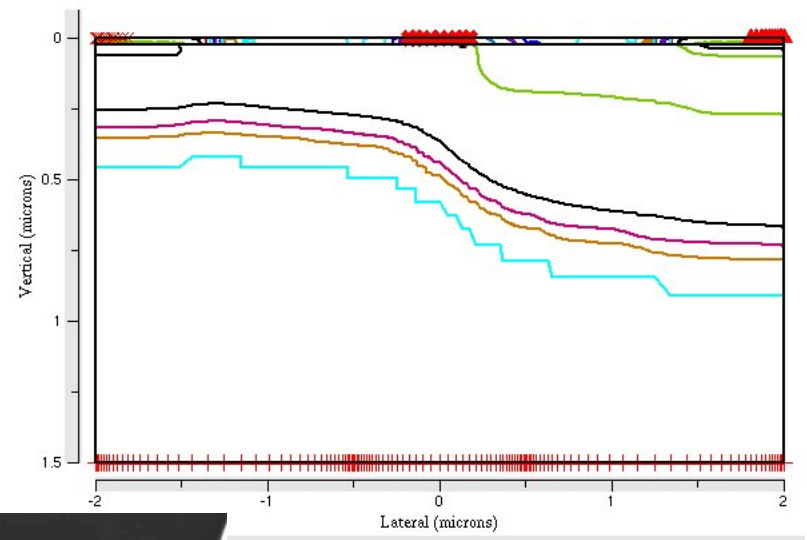
Inverse Piezoelectric Effect Calculation

- Electro-Mechanical Simulation with InversePiezo
- 25V Drain - above the del Alamo threshold



Off State

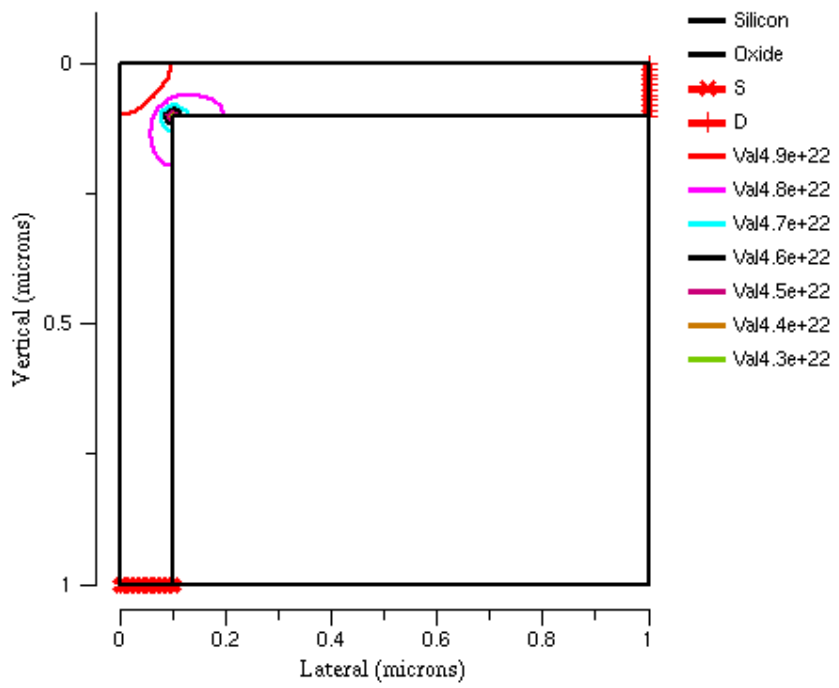




On State

Material Flow Simulation

- Crude electromigration simulation
- Density is lowest where field is highest (corner)
- Field driven kickout mechanism



Conclusions / Directions

- Experimentally Integrated
  - Failure Mechanism Identification feeds M&S
  - Electrical Measurement feeds Model Accuracy

- Direction
  - Integrate Pieces Discussed
  - Connect strain calculations to Temp, Traps
  - Work on Trap Generation - Bosman Connection